10556229

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1626GMS

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	NOV 21	CAS patent coverage to include exemplified prophetic substances identified in English-, French-, German-, and Japanese-language basic patents from 2004-present
NEWS 3	NOV 26	MARPAT enhanced with FSORT command
NEWS 4	NOV 26	CHEMSAFE now available on STN Easy
NEWS 5	NOV 26	Two new SET commands increase convenience of STN searching
NEWS 6	DEC 01	ChemPort single article sales feature unavailable
NEWS 7	DEC 12	GBFULL now offers single source for full-text coverage of complete UK patent families
NEWS 8	DEC 17	Fifty-one pharmaceutical ingredients added to PS
NEWS 9	JAN 06	The retention policy for unread STNmail messages will change in 2009 for STN-Columbus and STN-Tokyo
NEWS 10	JAN 07	WPIDS, WPINDEX, and WPIX enhanced Japanese Patent Classification Data
NEWS 11	FEB 02	Simultaneous left and right truncation (SLART) added for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS 12	FEB 02	GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS 13	FEB 06	Patent sequence location (PSL) data added to USGENE
NEWS 14	FEB 10	COMPENDEX reloaded and enhanced
NEWS 15	FEB 11	WTEXTILES reloaded and enhanced
NEWS 16	FEB 19	New patent-examiner citations in 300,000 CA/CAplus patent records provide insights into related prior art
NEWS 17	FEB 19	Increase the precision of your patent queries -- use terms from the IPC Thesaurus, Version 2009.01
NEWS 18	FEB 23	Several formats for image display and print options discontinued in USPATFULL and USPAT2
NEWS 19	FEB 23	MEDLINE now offers more precise author group fields and 2009 MeSH terms
NEWS 20	FEB 23	TOXCENTER updates mirror those of MEDLINE - more precise author group fields and 2009 MeSH terms
NEWS 21	FEB 23	Three million new patent records blast AEROSPACE into STN patent clusters
NEWS 22	FEB 25	USGENE enhanced with patent family and legal status display data from INPADOCDB
NEWS 23	MAR 06	INPADOCDB and INPAFAMDB enhanced with new display formats
NEWS 24	MAR 11	EPFULL backfile enhanced with additional full-text applications and grants

```
 NEWS 25  MAR 11  ESBIOBASE reloaded and enhanced
 NEWS 26  MAR 20  CAS databases on STN enhanced with new super role
                  for nanomaterial substances
 NEWS 27  MAR 23  CA/CAplus enhanced with more than 250,000 patent
                  equivalents from China

 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
specific topic.

  All use of STN is subject to the provisions of the STN customer
  agreement.  This agreement limits use to scientific research.  Use
  for software development or design, implementation of commercial
  gateways, or use of CAS and STN data in the building of commercial
  products is prohibited and may result in loss of user privileges
  and other penalties.

* * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:27:04 ON 25 MAR 2009

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files.  For example, the EXPAND
command can only be used to look at the index in a file which has an
index.  Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.22       0.22

FILE 'REGISTRY' ENTERED AT 10:27:18 ON 25 MAR 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2009 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   23 MAR 2009  HIGHEST RN 1125796-38-4
DICTIONARY FILE UPDATES:  23 MAR 2009  HIGHEST RN 1125796-38-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.
```

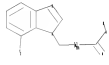
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

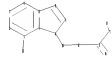
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10556229x.str





chain nodes :
10 11 12 13 14 15 21
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-21 6-10 10-11 11-12 12-13 12-15 13-14
ring bonds :
1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9
exact/norm bonds :
1-21 5-6 5-9 6-7 6-10 8-9 12-13 12-15
exact bonds :
10-11 11-12 13-14
normalized bonds :
1-2 1-7 2-3 3-4 4-8 7-8
isolated ring systems :
containing 1 :

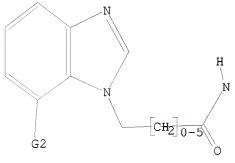
G1:H,Ak,CH3

G2:X,Ak,CN,NH2,NO2,Hy

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 21:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 H,Ak,Me

G2 X,Ak,CN,NH2,NO2,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 10:27:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2846 TO ITERATE

70.3% PROCESSED 2000 ITERATIONS 18 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 53720 TO 60120
PROJECTED ANSWERS: 209 TO 815

L2 18 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 10:27:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 56286 TO ITERATE

100.0% PROCESSED 56286 ITERATIONS 361 ANSWERS

SEARCH TIME: 00.00.04

L3 361 SEA SSS FUL L1

=> FIL HCAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	185.88	186.10

FILE 'HCAPLUS' ENTERED AT 10:27:51 ON 25 MAR 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 25 Mar 2009 VOL 150 ISS 13
FILE LAST UPDATED: 24 Mar 2009 (20090324/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 15 L3

=> s l4 and py<=2003
24034884 PY<=2003
L5 4 L4 AND PY<=2003

=> d l5 ibib abs hitstr tot

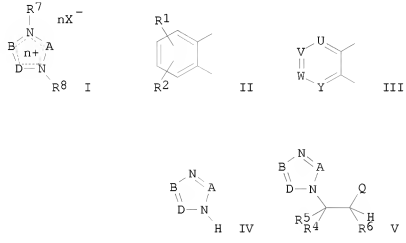
L5 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:	2000:219222 HCAPLUS
DOCUMENT NUMBER:	132:222537
TITLE:	Preparation of substituted nitrogen-containing heterocyclic compounds
INVENTOR(S):	Horvath, Andras; Salamon, Zoltan
PATENT ASSIGNEE(S):	Hung.
SOURCE:	Hung. Teljes, 21 pp. CODEN: HUXXBU
DOCUMENT TYPE:	Patent

LANGUAGE: Hungarian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
HU 78019	A2	19990528	HU 1995-962	19950331 <--
PRIORITY APPLN. INFO.:			HU 1995-962	19950331
OTHER SOURCE(S):	MARPAT 132:222537			

GI

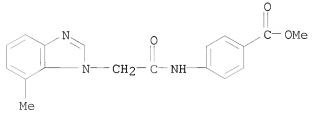


AB The title compds. [I; A = CR1, CR3; B = CR1; D = CR2, CR2:CR3, N; BD = II, III; R1-R3 = H, alkyl; U, V, W, Y, Z = (un)substituted Ph, NHCOalkyl, CO2alkyl, etc.; n = 0-1; X = Cl, Br, I, etc.; R7 = H, alkyl, heteroaryl; R8 = H, CR4R5CHR6Q; R4-R6 = H, alkyl, cycloalkyl, Q; Q = CN, CO2alkyl, COalkyl, etc.], useful as intermediates for biol. active compds., were prepared by reacting compound IV with olefin R4R5C:CR6Q followed by treatment of N-monoalkylated compound V with R7X.

IT 172839-71-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of substituted nitrogen-containing heterocyclic compds.)

RN 172839-71-3 HCAPLUS

CN Benzoic acid, 4-[[2-(7-methyl-1H-benzimidazol-1-yl)acetyl]amino]-, methyl ester (CA INDEX NAME)



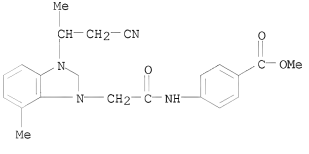
L5 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:866656 HCAPLUS
DOCUMENT NUMBER: 124:117179
ORIGINAL REFERENCE NO.: 124:21829a,21832a
TITLE: Michael adducts in the regioselective synthesis of N-substituted azoles
AUTHOR(S): Horvath, Andras
CORPORATE SOURCE: Alkaloida Chem. Co. Ltd., Tiszavasvari, Hung.
SOURCE: Synthesis (1995), (9), 1183-9
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:117179

AB Michael adducts of azoles (4-phenyl-, 4-methyl-, and 4-nitroimidazole, 4-methylbenzimidazole, 1,2,4-triazole, and theophylline) are shown to be valuable substrates for obtaining the N-substituted derivs. of the parent heterocycles by a quaternization-Hofmann elimination sequence. The effectiveness of the procedure is dependent on the regiochem. outcome of the 1st, N-protective step, i.e. the Michael addition By choosing the appropriate Michael acceptor, alkylating agent, and deprotection conditions, the thermodynamically less stable regioisomers of N-substituted azoles were obtained in high yields.

IT 172839-61-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-substituted azoles via regioselective Michael addition)

RN 172839-61-1 HCAPLUS

CN 1H-Benzimidazolium, 3-(2-cyano-1-methylethyl)-1-[2-[[4-(methoxycarbonyl)phenyl]amino]-2-oxoethyl]-7-methyl-, bromide (1:1) (CA INDEX NAME)

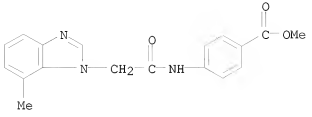


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

IT 172839-71-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation via regioselective Michael addition)

RN 172839-71-3 HCAPLUS

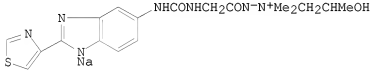
CN Benzoic acid, 4-[[2-(7-methyl-1H-benzimidazol-1-yl)acetyl]amino]-, methyl ester (CA INDEX NAME)



L5 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1982:510007 HCAPLUS
DOCUMENT NUMBER: 97:110007
ORIGINAL REFERENCE NO.: 97:18305a,18308a
TITLE: Benzimidazoles
INVENTOR(S): Jemison, Robert William; Beames, David John
PATENT ASSIGNEE(S): ICI Australia Ltd. , Australia
SOURCE: Pat. Specif. (Aust.), 56 pp.
CODEN: ALXXAP
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AU 519236	B2	19811119	AU 1978-35043	19770422 <--
AU 7835043	A	19791018		
PRIORITY APPLN. INFO.:			AU 1977-9860 A	19770422

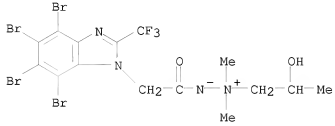
OTHER SOURCE(S): CASREACT 97:110007
GI



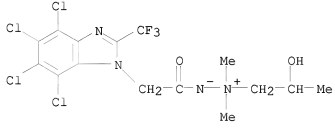
I

AB R[XN-N+R1R2R3]n [R = (un)substituted benzimidazolyl, R1-R3 = (un)substituted alkyl; X = CO, O2C, NHCO, X1CO, COX1CO, NHCOX1CO, CONHX1CO, SO2, 4-SC6H4O2C, NHCONHX1CO, 4-COC6H4O2C, 4-COC6H4NHCO, 4-SOC6H4CO, 4-COC6H4CO, 4-SOC6H4O2C; X1 = alkylene; n = 1-3] were prepared Thus 5-amino-2-(4-thiazolyl)benzimidazole was treated with OCNCH2CO2Me to give the 5-methoxycarbonylmethylureidobenzimidazole derivative which was treated with Me2NNH2 and propylene oxide to give I. At 50 mg/kg s.c. in sheep I reduced the fecal Hemonchus egg count from 800 to 0 on the 2nd day.
IT 82792-01-6P 82792-02-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 82792-01-6 HCAPLUS

CN Hydrazinium, 1-(2-hydroxypropyl)-1,1-dimethyl-2-[2-[4,5,6,7-tetrabromo-2-(trifluoromethyl)-1H-benzimidazol-1-yl]acetyl]-, inner salt (CA INDEX NAME)



RN 82792-02-7 HCAPLUS
CN Hydrazinium, 1-(2-hydroxypropyl)-1,1-dimethyl-2-[2-[4,5,6,7-tetrachloro-2-(trifluoromethyl)-1H-benzimidazol-1-yl]acetyl]-, inner salt (CA INDEX NAME)



L5 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1969:88247 HCAPLUS
DOCUMENT NUMBER: 70:88247
ORIGINAL REFERENCE NO.: 70:16521a,16524a
TITLE: Participation of the anilino group in peptide bond cleavage. Use of tert-butyl 3,5-dinitro-2-fluorocarbanilate as a peptide reagent
AUTHOR(S): Kirk, Kenneth L.; Cohen, Louis A.
CORPORATE SOURCE: Nat. Inst. of Allergy and Metab. Diseases, Nat. Inst. of Health, Bethesda, MD, USA
SOURCE: Journal of Organic Chemistry (1969), 34(2), 395-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Picramyl fluoride (3,5-dinitro-2-fluoroaniline) (I) was prepared by the SnCl2 reduction of picryl fluoride and by the Curtius rearrangement of 3,5-dinitro-2-fluorobenzoyl azide. Reaction of I with peptides (at pH 8) results in replacement of the F atom by the peptide N. Coupling is followed by rapid intramol. attack of the anilino group on the neighboring peptide bond (even at pH 8), resulting in cleavage of that bond and the formation of a dihydro-quinoxalinone derivative of the N-terminal amino acid. By use of I tert-BuO2C derivative, the coupling and cleavage steps can be

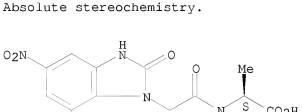
separated Removal of the blocking group by F3CCO2H is followed by rapid cyclization, both reactions proceeding quant. Sequencing of a polypeptide (e.g., oxidized insulin A chain) provides steadily decreasing yields of N-terminal derivs., due to benzimidazolinone formation during the coupling step. By kinetic anal., it is shown that the benzimidazolinone arises from attack of the 2,4-dinitroaniline anion on the adjacent tert-Bu carbanilate group.

IT 18646-10-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 18646-10-1 HCAPLUS

CN Alanine, N-[(5,7-dinitro-2-oxo-1-benzimidazolinyl)acetyl]-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d l4 ibib abs tot

L4 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:1372392 HCAPLUS

DOCUMENT NUMBER: 150:269

TITLE: Potent benzimidazolone-based CGRP receptor antagonists

AUTHOR(S): Theberge, Cory R.; Bednar, Rodney A.; Bell, Ian M.; Corcoran, Halea A.; Fay, John F.; Hershey, James C.; Johnston, Victor K.; Kane, Stefanie A.; Mosser, Scott; Salvatore, Christopher A.; Williams, Theresa M.; Zartman, C. Blair; Zhang, Xu-Fang; Graham, Samuel L.; Vacca, Joseph P.

CORPORATE SOURCE: Department of Medicinal Chemistry, Merck & Co., Inc., West Point, PA, 19486, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2008), 18(23), 6122-6125
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The previously disclosed spirohydantoin-based CGRP receptor antagonists were optimized for potency through modification of the benzimidazolone substituents. Compds. were identified which had minimal shift in the cAMP functional assay containing 50% human serum. Blockade of CGRP-mediated vasodilation was observed with these compds. in a rhesus pharmacodynamic assay and the in vivo potency correlated with the in vitro activity in the serum-shifted functional assay.

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:192495 HCAPLUS
DOCUMENT NUMBER: 148:239209
TITLE: Benzimidazole derivatives as vanilloid receptor antagonists, their preparation, pharmaceutical compositions, and use in therapy
INVENTOR(S): Brown, William; Johnstone, Shawn; Labrecque, Denis
PATENT ASSIGNEE(S): AstraZeneca AB, Swed.
SOURCE: PCT Int. Appl., 136pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2008018827	A1	20080214	WO 2007-SE720		20070810
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 20080221188	A1	20080911	US 2007-836221		20070809
AU 2007282186	A1	20080214	AU 2007-282186		20070810
PRIORITY APPLN. INFO.:			US 2006-837249P	P	20060811
			WO 2007-SE720	W	20070810

OTHER SOURCE(S): MARPAT 148:239209
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention provides benzimidazole derivs. of formula I, which are antagonists of vanilloid receptor 1 (VR-1). In compds. I, R1 is halo, cyano, or acetyl; R2 is H or Me; R3 is H or halo; R4 and R5 are independently selected from Me and Et, or R4 and R5, together with the carbon atom to which they are attached, form C3-6 cycloalkyl or a 5- or 6-membered heterocyclyl; n is 0-2; and each R6 is independently selected from halo, Me, and Et. The invention also relates to the preparation of I, pharmaceutical compns. comprising a compound according to formula I and a pharmaceutically acceptable carrier, as well as to the use of the compns. for the treatment of disorders responding to VR-1 inhibition, such as osteoarthritis, chronic tendinitis, pelvic pain, peripheral neuropathy, gastroesophageal reflux disease, irritable bowel syndrome, and overactive bladder. Substitution of 1,2,3-trifluoro-4-nitrobenzene with ethanolamine followed by hydrogenation, heterocyclization with formic acid, and oxidation

gave benzimidazole II. Double α-methylation of (4-bromophenyl)acetonitrile followed by lithiation, condensation with N-methoxy-N-methyl-acetamide, and reductive amination resulted in the formation of amine III, which underwent amidation with II and chiral HPLC separation to give IV and its enantiomer. Some compds. of the invention express antagonist activity to VR-1 below 100 nM (no specific data).

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:1177157 HCAPLUS
DOCUMENT NUMBER: 147:448786
TITLE: Preparation of oxadiazole compounds as S1P1 agonists
INVENTOR(S): Harada, Hironori; Hattori, Kazuyuki; Fujita, Kazuya; Morita, Masataka; Imada, Sunao; Abe, Yoshito; Itani, Hiromichi; Morokata, Tatsuaki; Tsutsumi, Hideo
PATENT ASSIGNEE(S): Astellas Pharma Inc., Japan
SOURCE: PCT Int. Appl., 105pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007116866	A1	20071018	WO 2007-JP57414	20070402
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2007236707	A1	20071018	AU 2007-236707	20070402
CA 2648303	A1	20071018	CA 2007-2648303	20070402
EP 2003132	A1	20081217	EP 2007-740850	20070402
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR				
US 20090076070	A1	20090319	US 2008-244102	20081002
NO 2008004618	A	20081217	NO 2008-4618	20081031
KR 2009007740	A	20090120	KR 2008-726792	20081031

PRIORITY APPLN. INFO.:

JP 2006-102544	A	20060403
JP 2006-276693	A	20061010
JP 2006-279227	A	20061012
WO 2007-JP57414	W	20070402

OTHER SOURCE(S): MARPAT 147:448786
GI

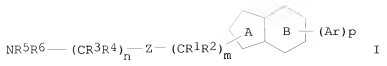
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [ring A = Q1, etc.; X = single bond, -CH2-, -NR3-, etc.; R1 = -H, halo, aryl, etc.; R2 = -CN, -O-alkyl, -CHO, etc.; R3 = -H; R3 and R1, together with the nitrogen to which they are attached, may form morpholino, 1-pyrrolidinyl or 3,4-dihydropiperidin-1-yl (sic); when X is a single bond, R1 and R2 may combine to form a 5-membered ring (wherein 5-membered ring is optionally substituted with alkyl); R4 = Q2, etc. (one bond from Q2 is linked to oxadiazolyl ring); R5 = -H, -CN, -NHRx, etc.; Rx = -H, -OH, (un)protected amino, etc.] or their pharmaceutically acceptable salts were prepared For example, reaction of 1,3-difluoropropan-2-ol with NaH followed by in-situ treatment with 2-[4-[5-(3-chloro-4-fluorophenyl)-1,2,4-oxadiazol-3-yl]-1H-indol-1-yl]acetamide afforded compound II. The exemplified compound II showed the S1P1 agonistic activity with EC50 = 1.2 nM. Compds. I are claimed useful for the treatment of autoimmune disease, multiple sclerosis, etc.
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

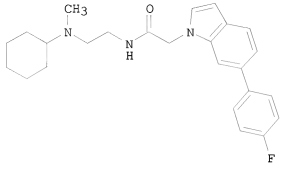
L4 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:1146647 HCAPLUS
DOCUMENT NUMBER: 147:448636
TITLE: Preparation of indoles, indazoles, benzimidazoles and their analogs as chemokine receptor CXCR4 and CCR7 inhibitors
INVENTOR(S): Thomas, William D.; Leleti, Manmohan Reddy; Pennell, Andrew M. K.
PATENT ASSIGNEE(S): Chemocentryx, Inc., USA
SOURCE: PCT Int. Appl., 142pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007115231	A2	20071011	WO 2007-US65729	20070330
WO 2007115231	A3	20080717		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
US 20070275965	A1	20071129	US 2007-731695	20070330

PRIORITY APPLN. INFO.: US 2006-787925P P 20060330
OTHER SOURCE(S): MARPAT 147:448636
GI



I



II

AB Title compds. I [wherein R1 - R4 independently = H, halo, alkyl, etc.; R5, R6 independently = H, alkyl, cycloalkyl, etc.; Z = C(O), C(O)O, CONH, etc.; m, n = 1-6; ring A = (un)substituted fused 5-membered heteroaryl or heterocycloalkyl; ring B = (un)substituted fused 6-membered (hetero)aryl or (hetero)cycloalkyl; Ar = (un)substituted (hetero)aryl; p = 0-1] and pharmaceutically acceptable salts, hydrates and N-oxides thereof, which can inhibit the binding of the SDF-1 chemokine to the chemokine receptor CXCR4 and/or the binding of the SDF-1 or I-TAC chemokines to the chemokine receptor CCXCKR2 (CXCR7), were prepared For instance, II was synthesized and had IC50 < 1 μM for both CXCR4 and CXCR7 receptors in chemotaxis or binding assays. The invented compds. and their pharmaceutical compns. are useful for the treatment of CXCR4-mediated diseases or conditions.

L4 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:703476 HCAPLUS
DOCUMENT NUMBER: 147:118229
TITLE: Benzimidazole compounds and their preparation, pharmaceutical compositions and use in the treatment of VR1-mediated diseases
INVENTOR(S): Besidski, Yevgeni; Griffin, Andrew; Labrecque, Denis; Johnstone, Shawn; Jones, Paul; Kers, Inger; Nyloef, Martin; Skogholm, Karin
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 89pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007073303	A2	20070628	WO 2006-SE1467	20061221
WO 2007073303	A3	20070830		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

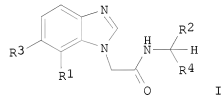
GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN,
KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK,
MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO,
RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT,
TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

AU	2006327320	A1	20070628	AU 2006-327320	20061221
CA	2634804	A1	20070628	CA 2006-2634804	20061221
US	20080171770	A1	20080717	US 2006-614346	20061221
EP	1966156	A2	20080910	EP 2006-835882	20061221
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS				
IN	2008DN05119	A	20080926	IN 2008-DN5119	20080613
MX	2008007837	A	20080626	MX 2008-7837	20080617
KR	2008080212	A	20080902	KR 2008-717908	20080722
NO	2008003246	A	20080911	NO 2008-3246	20080722
CN	101389610	A	20090318	CN 2006-80053368	20080825

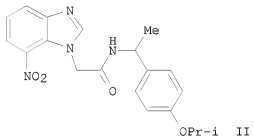
PRIORITY APPLN. INFO.: US 2005-753604P P 20051223
WO 2006-SE1467 W 20061221

OTHER SOURCE(S): MARPAT 147:118229

GI



I



II

AB The invention relates to new compds. formula I or salts, solvates or solvated salts thereof, processes for their preparation and to intermediates used in the preparation thereof, pharmaceutical compns. containing said compds. and
to the use of said compds. in therapy. Compds. of formula II wherein R1 is NO2, CN, halo, and acetyl; R2 is (un)substituted Ph, (un)substituted

heteroaryl, (un)substituted PhCH2, and (un)substituted PhOCH2; R3 is H and F; R4 is Me, MeOCO, and Et; R2R4 taken together may form (mono/bi)cyclic ring; and their salts, solvates and solvated salts thereof, are claimed. Example compound II was prepared by a general procedure (procedure given). All the invention compds. were evaluated for their VR1 inhibitory activity.

L4 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:48925 HCAPLUS
DOCUMENT NUMBER: 146:308386
TITLE: In Silico Binding Free Energy Predictability by Using the Linear Interaction Energy (LIE) Method: Bromobenzimidazole CK2 Inhibitors as a Case Study
AUTHOR(S): Bortolato, A.; Moro, S.
CORPORATE SOURCE: Molecular Modeling Section, Department of Pharmaceutical Sciences, University of Padova, Padua, I-35131, Italy
SOURCE: Journal of Chemical Information and Modeling (2007), 47(2), 572-582
CODEN: JCISD8; ISSN: 1549-9596
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Protein kinase CK2 is essential for cell viability, and its control regards a broad series of cellular events such as gene expression, RNA, and protein synthesis. Evidence of its involvement in tumor development and viral replication indicates CK2 as a potential target of antineoplastic and antiviral drugs. In this study the Linear Interaction Energy (LIE) Method with the Surface Generalized Born (SGB) continuum solvation model was used to study several bromobenzimidazole CK2 inhibitors. This methodol., developed by Aqvist, finds a plausible compromise between accuracy and computational speed in evaluating binding free energy (AGbind) values. In this study, two different free binding energy models, named "CK2scoreA" and "CK2scoreB", were developed using 22 inhibitors as the training set in a stepwise approach useful to appropriately select both the tautomeric form and the starting binding position of each inhibitor. Both models are statistically acceptable. Indeed, the better one is characterized by a correlation coefficient (r2) of 0.81, and the predictive accuracy was 0.65 kcal/mol. The corresponding validation, using an external test set of 16 analogs, showed a correlation coefficient (q2) of 0.68 and a prediction root-mean-square error of 0.78 kcal/mol. In this case, the LIE approach has been proved to be an efficient methodol. to rationalize the difference of activity, the key interactions, and the different possible binding modes of this specific class of potent CK2 inhibitors.
REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

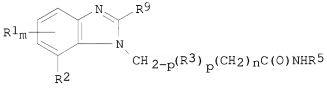
L4 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:298140 HCAPLUS
DOCUMENT NUMBER: 144:331439
TITLE: Preparation of benzimidazol-1-yl-substituted alkanoic acid amides as vanilloid receptor 1 antagonists with analgesic and other therapeutic potential
INVENTOR(S): Besidski, Yevgeni; Kers, Inger; Nyloef, Martin; Slaitas, Andis
PATENT ASSIGNEE(S): AstraZeneca AB, Swed.

SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006033620	A1	20060330	WO 2005-SE1364	20050919
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2005285656	A1	20060330	AU 2005-285656	20050919
CA 2577818	A1	20060330	CA 2005-2577818	20050919
EP 1797067	A1	20070620	EP 2005-783773	20050919
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR				
CN 101023071	A	20070822	CN 2005-80031737	20050919
JP 2008513443	T	20080501	JP 2007-532288	20050919
BR 2005015429	A	20080722	BR 2005-15429	20050919
IN 2007DN01584	A	20070803	IN 2007-DN1584	20070227
MX 2007003119	A	20070524	MX 2007-3119	20070315
US 20080015222	A1	20080117	US 2007-575635	20070320
KR 2007056104	A	20070531	KR 2007-706447	20070321
NO 2007002005	A	20070615	NO 2007-2005	20070419

PRIORITY APPLN. INFO.: SE 2004-2284 A 20040921
WO 2005-SE1364 W 20050919

OTHER SOURCE(S): CASREACT 144:331439; MARPAT 144:331439
GI



I

AB The present invention relates to benzimidazol-1-yl-substituted alkanoic acid amides (shown as I; variables defined below; e.g. 2-(7-amino-1H-benzimidazol-1-yl)-N-(4-tert-butylbenzyl)acetamide (II)) or salts, solvates or solvated salts thereof, processes for their preparation and to new intermediates used in the preparation thereof, pharmaceutical compns. containing said compds. and to the use of said compds. in therapy. For I: R1 is H, NO2, halo, NR6R7, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C1-6

haloalkyl, C1-6 haloalkyl O, R6OC0-6 alkyl, R6CO, R6OCO, or CONR6R7; m = 0-3; R2 is H, NO2, halo, NR6R7, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C1-6 haloalkyl, C1-6 haloalkyl O, cyano, R6OC0-6 alkyl, R6CO, R6OCO, R6CONR7, R6R7NCO, R8SO2, R8SO2HN, aryl C0-6 alkyl or heteroaryl C0-6 alkyl; R3 and R9 = H or C1-4 alkyl; R2 and R3 optionally form a ring; p = 0-2; n = 0, 2, 3, or 4; R5 is C1-10 alkyl, C6-10 aryl C0-6 alkyl, C3-7 cycloalkyl C0-6 alkyl, or C5-6 heteroaryl C0-6 alkyl, whereby any aryl, heteroaryl,or cycloalkyl may be fused with aryl, heteroaryl, C3-7 cycloalkyl, or C3-7 heterocycloalkyl, and which R5 may be substituted with ≥1 A; A is H, OH, NO2, cyano, R6CO, R6O(CO), halo, C1-6 alkyl, NR6R7, C1-6 haloalkyl, C1-6 haloalkyl O, R6OC0-6 alkyl, hydroxy C1-6 alkyl, R8SO2, R8SO2HN, C5-6 aryl O or CONR6R7; R6 and R7 = H or C1-6 alkyl; and R8 is NR6R7 or C1-4 alkyl. Although the methods of preparation are not claimed, prepns. and/or characterization data for 65 examples of I are included. Many of the examples were prepared from a 7-substituted (1H-benzimidazol-1-yl)acetic acid (prepns. described) and an amine in MeCN in the presence of Et3N and O-(7-azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate. IC50 values for 4 examples of I acting as antagonists of the vanilloid receptor 1 in the presence of agonists like capsaicin or 2-(morpholino)ethanesulfonic acid are tabulated.

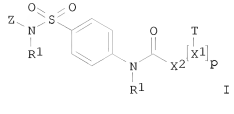
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN

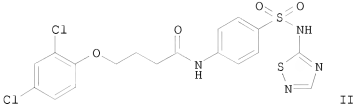
ACCESSION NUMBER: 2006:103871 HCAPLUS
DOCUMENT NUMBER: 144:192238
TITLE: Preparation of N-(4-sulfamoylphenyl) amides as inhibitors of voltage-gated sodium channels
INVENTOR(S): Gonzalez, Jesus E.; Termin, Andreas P.; Martinborough, Esther; Zimmerman, Nicole
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 353 pp., Cont.-in-part of U.S. Ser. No. 914,988.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20060025415	A1	20060202	US 2005-60719		20050217
US 20050137190	A1	20050623	US 2004-914988		20040809
PRIORITY APPLN. INFO.:			US 2003-493659P	P	20030808
			US 2004-584717P	P	20040704
			US 2004-914988	A2	20040809

OTHER SOURCE(S): CASREACT 144:192238; MARPAT 144:192238
GI



I



II

AB The title compds. I [R1 = H, (un)substituted alkyl; X1 = O, S, (un)substituted NH; p = 0-1; X2 = (un)substituted alkylene; Z = thiazolyl, imidazolyl, oxazolyl, etc.; T = (un)substituted Ph, 8-14 membered (non)aromatic bicyclic or tricyclic ring having 0-5 heteroatoms selected from O, S, N, NH, SO, SO2, etc.], useful as inhibitors of voltage-gated sodium channels, were prepared E.g., a multi-step synthesis of II, starting from 2,4-dichlorophenol and Et 4-bromobutyrate, was given. The compds. I were found to inhibit voltage-gated sodium channels at 25.0 μM or less. I were also found possess desired N-type calcium channel modulation activity and selectivity (no data given). The invention also provides pharmaceutically acceptable compsns. comprising the compds. I and methods of using the compsns. in the treatment of various disorders.

L4 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1103734 HCAPLUS
DOCUMENT NUMBER: 143:386764
TITLE: Preparation of aniline derivatives as kininogenase inhibitors
INVENTOR(S): Tokumasu, Munetaka; Sugiki, Masayuki; Hirashima, Haruko; Matsumoto, Hideki; Yoshimura, Toshihiko; Nogi, Yasuko; Takahashi, Mitsuo; Kitazawa, Manabu; Oonuki, Akiko; Fukuchi, Naoyuki; Shima, Yoichiro
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan; et al.
SOURCE: PCT Int. Appl., 137 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095327	A1	20051013	WO 2005-JP6834	20050331

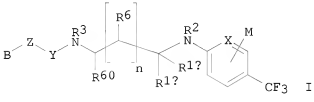
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,
SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG

EP 1736465 A1 20061227 EP 2005-728768 20050331
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA,
HR, LV, MK, YU

US 20070066586 A1 20070322 US 2006-537139 20060929
PRIORITY APPLN. INFO.: JP 2004-107368 A 20040331
WO 2005-JP6834 W 20050331

OTHER SOURCE(S): MARPAT 143:386764
GI



AB The title compds., e.g. I [X = C, N ; M = H, halo, (un)substituted alkyl, etc.; Z = single bond, CH:CH, CO, etc.; B = H, (un)substituted alkyl, etc.; R3 = H, (un)substituted alkyl, (un)substituted aryl; further detail on R3 is given; Y = CO, SO2; R1a, R1b = H, (un)substituted alkyl, (un)substituted aryl; further detail on R1a and R1b is given; R2 = H, alkyl; further detail related to R1a, R1b and R2 is given; n = 0 or 1; R6 and R60 = H, (un)substituted alkyl, amino, etc.], are prepared Thus, N-((2R)-3-methyl-2-[[4-(trifluoromethyl)phenyl]-amino]butyl)-2-phenylacetamide CF3CO2H salt was prepared in 3 steps from 4-trifluoromethyliodobenzene and D-valine. In an in vitro test for tissue kallikrein inhibiting activity, compds. of this invention showed pIC50 values of 6.51 to 7.70. In a test for analgesic activity using mice, compds. of this invention at 30 mg/kg orally showed activity equal to that of indomethacin at 10 mg/kg orally.

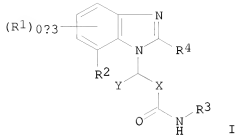
L4 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:1019865 HCAPLUS
DOCUMENT NUMBER: 142:6536
TITLE: A preparation of benzimidazole derivatives, useful as inhibitors of vanilloid receptor 1
INVENTOR(S): Besidski, Yevgeni; Kers, Inger; Nyloef, Martin; Rotticci, Didier; Slaitas, Andis; Svensson, Mats
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

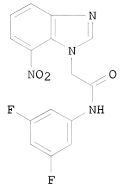
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004100865	A2	20041125	WO 2004-SE738	20040513
WO 2004100865	A3	20050120		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004238177	A1	20041125	AU 2004-238177	20040513
AU 2004238177	B2	20080424		
CA 2525628	A1	20041125	CA 2004-2525628	20040513
EP 1626964	A2	20060222	EP 2004-732865	20040513
EP 1626964	B1	20090121		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
BR 2004010316	A	20060523	BR 2004-10316	20040513
CN 1784387	A	20060607	CN 2004-80012619	20040513
CN 100413849	C	20080827		
JP 2006528971	T	20061228	JP 2006-532186	20040513
RU 2337098	C2	20081027	RU 2005-136529	20040513
CN 101328150	A	20081224	CN 2008-10136051	20040513
AT 421506	T	20090215	AT 2004-732865	20040513
IN 2005DN04859	A	20071012	IN 2005-DN4859	20051024
US 20060287377	A1	20061221	US 2005-556229	20051109
MX 2005012247	A	20060210	MX 2005-12247	20051114
NO 2005005977	A	20060216	NO 2005-5977	20051215
AU 2008203305	A1	20080814	AU 2008-203305	20080724

PRIORITY APPLN. INFO.:	SE 2003-1446	A	20030516
	SE 2004-43	A	20040112
	AU 2004-238177	A3	20040513
	CN 2004-80012619	A3	20040513
	WO 2004-SE738	W	20040513

OTHER SOURCE(S): MARPAT 142:6536
GI



I



II

AB The invention relates to a preparation of new benzimidazole derivs. of formula I [wherein: X is CH2 or (CH2)2-4; Y is H or (alkyl)0-2; R1 is H, NO2, halogen, alk(en/yn)yl, or (H/alkyl)C(O), etc.; R2 is NO2, halogen, alk(en/yn)yl, or haloalkyl, etc.; R3 is alkyl, arylalkyl, cycloalkylalkyl, or heteroarylalkyl, etc.; R4 is H or alkyl], useful as inhibitors of vanilloid receptor 1 (VR 1). For instance, benzimidazole derivative II was prepared via amidation of 2-(7-nitro-1H-benzimidazol-1-yl)acetic acid by 3,5-difluoroaniline. The prepared title compds. were screened in fluorometric image plate reader assay (hVR1 FLIPR) (II, IC50 = 50 nM).

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:920737 HCAPLUS
DOCUMENT NUMBER: 142:247
TITLE: Optimization of Protein Kinase CK2 Inhibitors Derived from 4,5,6,7-Tetrabromobenzimidazole
AUTHOR(S): Pagano, Mario A.; Andrzejewska, Mariola; Ruzzene, Maria; Sarno, Stefania; Cesaro, Luca; Bain, Jenny; Elliott, Matthew; Meggio, Flavio; Kazimierczuk, Zygmunt; Pinna, Lorenzo A.
CORPORATE SOURCE: Dipartimento di Chimica Biologica, Universita di Padova, Padua, Italy
SOURCE: Journal of Medicinal Chemistry (2004), 47(25), 6239-6247
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:247

AB Casein kinase 2 (CK2) is a ubiquitous, essential, and highly pleiotropic protein kinase whose abnormally high constitutive activity is suspected to underlie its pathogenic potential in neoplasia and infective diseases. Thus, CK2 inhibitors designed to dissect the signaling pathways affected by this kinase, in perspective, may give rise to pharmacol. tools. One of the most successful CK2 inhibitors is TBB (4,5,6,7-tetrabromobenzotriazole). Here we show that its inhibitory properties can be markedly improved by generating adducts in which N2 is replaced by a carbon atom bound to a variety of polar functions. The most efficient inhibitor is 4,5,6,7-tetrabromo-2-(dimethylamino)benzimidazole (2c) followed by the methylsulfanyl (8), isopropylamino (2e), and amino (2a) congeners. All these compds. display Ki values <100 nM (40 nM in the case of 2c). 2C induces apoptosis of Jurkat cells more readily than TBB (DC50 value 2.7 vs 17 μM) and, unlike TBB, it does not display any side effect on mitochondria polarization up to 10 μM concentration Mol. modeling of the CK2-2c complex, based on the crystal structure of the CK2-TBB complex suggests that a number of addnl. apolar contacts between its two Me groups and hydrophobic residues nearby could account for its superior inhibitory properties. Consequently, 2c is even more susceptible than TBB to mutations of the unique hydrophobic residues V66 and/or I174 to alanine. We propose to adopt 2c as first choice CK2 inhibitor instead of TBB, especially for in cell studies.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:219222 HCAPLUS

DOCUMENT NUMBER: 132:222537

TITLE: Preparation of substituted nitrogen-containing heterocyclic compounds

INVENTOR(S): Horvath, Andras; Salamon, Zoltan

PATENT ASSIGNEE(S): Hung.

SOURCE: Hung. Teljes, 21 pp.
CODEN: HUXXBU

DOCUMENT TYPE: Patent

LANGUAGE: Hungarian

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
HU 78019	A2	19990528	HU 1995-962	19950331

PRIORITY APPLN. INFO.: HU 1995-962 19950331

OTHER SOURCE(S): MARPAT 132:222537

GI


I


II


III


IV V

AB The title compds. [I; A = CR1, CR3; B = CR1; D = CR2, CR2:CR3, N; BD = II, III; R1-R3 = H, alkyl; U, V, W, Y, Z = (un)substituted Ph, NHCOalkyl, CO2alkyl, etc.; n = 0-1; X = Cl, Br, I, etc.; R7 = H, alkyl, heteroaryl; R8 = H, CR4R5CHR6Q; R4-R6 = H, alkyl, cycloalkyl, Q; Q = CN, CO2alkyl, COalkyl, etc.], useful as intermediates for biol. active compds., were prepared by reacting compound IV with olefin R4R5C:CR6Q followed by treatment of N-monoalkylated compound V with R7X.

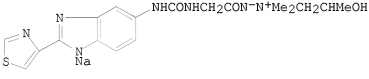
L4 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:866656 HCAPLUS
DOCUMENT NUMBER: 124:117179
ORIGINAL REFERENCE NO.: 124:21829a,21832a
TITLE: Michael adducts in the regioselective synthesis of N-substituted azoles
AUTHOR(S): Horvath, Andras
CORPORATE SOURCE: Alkaloida Chem. Co. Ltd., Tiszavasvari, Hung.
SOURCE: Synthesis (1995), (9), 1183-9
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:117179
AB Michael adducts of azoles (4-phenyl-, 4-methyl-, and 4-nitroimidazole, 4-methylbenzimidazole, 1,2,4-triazole, and theophylline) are shown to be valuable substrates for obtaining the N-substituted derivs. of the parent heterocycles by a quaternization-Hofmann elimination sequence. The effectiveness of the procedure is dependent on the regiochem. outcome of the 1st, N-protective step, i.e. the Michael addition By choosing the appropriate Michael acceptor, alkylating agent, and deprotection conditions, the thermodynamically less stable regioisomers of N-substituted azoles were obtained in high yields.

L4 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1982:510007 HCAPLUS
DOCUMENT NUMBER: 97:110007
ORIGINAL REFERENCE NO.: 97:18305a,18308a

TITLE: Benzimidazoles
INVENTOR(S): Jemison, Robert William; Beames, David John
PATENT ASSIGNEE(S): ICI Australia Ltd. , Australia
SOURCE: Pat. Specif. (Aust.), 56 pp.
CODEN: ALXXAP
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AU 519236	B2	19811119	AU 1978-35043	19770422
AU 7835043	A	19791018		
PRIORITY APPLN. INFO.:			AU 1977-9860 A	19770422

OTHER SOURCE(S): CASREACT 97:110007
GI



I

AB R[XN-N+R1R2R3]n [R = (un)substituted benzimidazolyl, R1-R3 = (un)substituted alkyl; X = CO, O2C, NHCO, X1CO, COX1CO, NHCOX1CO, CONHX1CO, SO2, 4-SC6H4O2C, NHCONHX1CO, 4-COC6H4O2C, 4-COC6H4NHCO, 4-SOC6H4CO, 4-COC6H4CO, 4-SOC6H4O2C; X1 = alkylene; n = 1-3] were prepared Thus 5-amino-2-(4-thiazolyl)benzimidazole was treated with OCNCH2CO2Me to give the 5-methoxycarbonylmethylureidobenzimidazole derivative which was treated with Me2NNH2 and propylene oxide to give I. At 50 mg/kg s.c. in sheep I reduced the fecal Hemonchus egg count from 800 to 0 on the 2nd day.

L4 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1969:88247 HCAPLUS
DOCUMENT NUMBER: 70:88247
ORIGINAL REFERENCE NO.: 70:16521a,16524a
TITLE: Participation of the anilino group in peptide bond cleavage. Use of tert-butyl 3,5-dinitro-2-fluorocarbanilate as a peptide reagent
AUTHOR(S): Kirk, Kenneth L.; Cohen, Louis A.
CORPORATE SOURCE: Nat. Inst. of Allergy and Metab. Diseases, Nat. Inst. of Health, Bethesda, MD, USA
SOURCE: Journal of Organic Chemistry (1969), 34(2), 395-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Picramyl fluoride (3,5-dinitro-2-fluoroaniline) (I) was prepared by the SnCl2 reduction of picryl fluoride and by the Curtius rearrangement of 3,5-dinitro-2-fluorobenzoyl azide. Reaction of I with peptides (at pH 8) results in replacement of the F atom by the peptide N. Coupling is followed by rapid intramol. attack of the anilino group on the neighboring peptide bond (even at pH 8), resulting in cleavage of that bond and the

formation of a dihydro-quinoxalinone derivative of the N-terminal amino acid. By use of I tert-BuO2C derivative, the coupling and cleavage steps can be separated Removal of the blocking group by F3CCO2H is followed by rapid cyclization, both reactions proceeding quant. Sequencing of a polypeptide (e.g., oxidized insulin A chain) provides steadily decreasing yields of N-terminal derivs., due to benzimidazolinone formation during the coupling step. By kinetic anal., it is shown that the benzimidazolinone arises from attack of the 2,4-dinitroaniline anion on the adjacent tert-Bu carbanilate group.

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	87.51	273.61

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-15.58	-15.58

STN INTERNATIONAL LOGOFF AT 10:32:08 ON 25 MAR 2009